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THE DOE VADOSE ZONE SCIENCE AND TECHNOLOGY ROADMAP:

A National Program to Address Characterization, Monitoring and Simulation of Subsurface Contaminant Fate and Transport

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ABSTRACT

The vadose zone comprises the region lying between the earth's surface and the top of the regional seasonal aquifer. Until recently contamination in the vadose zone was believed to remain relatively immobile. Thus, little attention was paid to understanding the nature of the vadose zone or the potential pathways for contaminants to migrate through it to the water table or other accessible environments. However, recent discoveries of contaminants migrating considerable distances through the vadose zone at several Department of Energy (DOE) sites have changed many assumptions both about the nature and function of the vadose zone and the importance we place on understanding this region.

As a result of several vadose zone surprises, DOE Environmental Management (EM) tasked the Idaho National Engineering and Environmental Laboratory (INEEL) to lead the development of a vadose zone science and technology roadmap. The roadmap is focused on identifying research spanning the next 25 years necessary to be able to better predict the fate and transport of contaminants in the vadose zone. This in turn will provide the basis for reducing scientific uncertainty in environmental remediation and, especially, vadose zone related long-term stewardship decisions across the DOE complex. Vadose zone issues are now recognized as a national problem affecting other federal agencies as well as state and municipal sites with similar problems.

Over the next few decades, dramatic and fundamental advances in computing, communication, electronics and micro-engineered systems will transform our understanding of many aspects of the scientific and technical challenges we face today. The roadmap will serve to develop a common perspective on possible future science and technology needs in an effort to help make better R&D investment decisions.

INTRODUCTION

The vadose zone science and technology roadmap (http://vadosezone.inel.gov/) considers the research and development (R&D) that will improve predictions of fate and transport of contaminants in the vadose zone, and thus reduce uncertainty in environmental decision-making. Science and technology roadmap development is a form of strategic technology planning used by an increasing number of companies, industries, and U.S. government agencies. The purpose of science and technology roadmaps is to develop a common perspective on possible future science and technology needs in an effort to help make better R&D investment decisions. Science and technology roadmaps serve as pathways to the future. They call attention to future needs for development in underpinning science and applied technology, provide a structure for organizing technology forecasts and programs, and communicate scientific technological needs and expectations among end-users and the R&D community.

> "It is notable that most major DOE contaminated sites are complex due to the geology and hydrology… of particular complexity is the unsaturated, or vadose zone." (1:79)

The DOE is particularly concerned about vadose zone issues. It has conducted energy research and weapons development and production at facilities in 31 states and in Puerto Rico. Toxic chemicals generated at these sites have been introduced into the underlying soils and aquifers as a result of a number of historical and current practices. At present, more than six billion cubic meters of subsurface media at 134 sites are contaminated. Of this approximately 700 million cubic meters is groundwater contaminated with organic wastes (e.g., solvents, fuels, PCBs), radioactive waste, or mixed (chemical and radioactive) radioactive waste (2). Typically, the groundwater contamination results from the migration of contaminants through the vadose zone. Today, some 60 million cubic meters of soil and rock comprising the vadose zone are contaminated, mostly with radioactive waste or mixed low-level radioactive waste. In addition, similar, non-radioactive, situations exist at other federal, state and municipal waste management facilities.

Anticipating the failure of some aspect of a long-term remediation or stewardship solution in the vadose zone is not unreasonable. Recent evidence indicates that hazardous and radioactive chemicals have migrated unexpectedly through the vadose zone at multiple DOE facilities (3). For example, at the Hanford 200 Area tank farm, technetium-99 migrated to ground water through 200 to 300 feet of what was previously believed to be highly sorptive material that would have prevented such migration. At Los Alamos National Laboratory, plutonium and americium were discovered 100 feet beneath a liquid waste impoundment where nuclide transport was believed to be dominated by sorption and thus radionuclide migration should have been very limited. At the Sandia National Laboratory TCE from a landfill has been discovered at depths of 500 feet in an area of very dry soil and low recharge. At the high-level radioactive waste disposal repository in the dry desert climate of Yucca Mountain, modern tracers, bomb pulse chlorine-36 and tritium, were found in fractured tuff at depths of as much as 1200 feet, suggesting rapid recharge along preferential pathways.

THE NEED FOR A NATIONAL RESPONSE

These surprises, and many others across the U.S., are clear indications that our current understanding and capabilities related to the vadose zone are inadequate. Our ability to characterize the spatial distribution of chemicals and their migration pathways is quite limited (4). The state-of-the-practice in vadose zone monitoring to detect chemical migration is limited primarily to in situ samplers that retrieve pore-water only from limited volumes of relatively wet soils, and to geophysical methods which only indirectly measure waste movement. There is no technology available to ensure detection of migration via discrete, narrow fingers in unsaturated porous media, or to sample fluids coating only portions of fracture surfaces, or to collect colloidal particles from the pore water in the vadose zone.

> "…support for basic scientific research aimed at improved understanding of sites and the fate and transport of residual contaminants on them…(is a) component of a comprehensive stewardship program…" (1:49)

In addition, field investigations often reveal that the extent of chemical migration is poorly predicted with mathematical models of flow and transport in the vadose zone. This record may be attributed to incomplete understanding or unrecognized physical/chemical/ biological processes; insufficient or inaccurate characterization of the processes or site properties; and inadequate or inaccurate numerical models. At present, there is no single predictive tool that has been demonstrated to reliably simulate fate and transport of organic and inorganic chemicals and radionuclides in vadose zones comprised of porous and fractured media under variably saturated conditions

The inability to explain basic subsurface processes and predict contaminant fate and transport in the vadose zone have led regulators to fall back on the most conservative expectations: all contaminants will move rapidly through the vadose zone to the groundwater. In the late 1960s travel time of C-14 from the surface to ground water at the INEEL was estimated at 80,000 years. Today the estimates are closer to 50 years. Similar foreshortening of travel time predictions for other contaminants has also occurred. Despite these dramatic changes in expectations, many in the scientific/technical community assert that we are no more certain of our current predictions than we were of those made three decades ago.

> "The relatively high likelihood that institutional management measures will fail at some point underscores the need to assure that decisions made in the near term are based on the best available science. Where deficiencies in scientific understanding that inhibit present-day planning are recognized, incorporating strategies for improving the scientific and technical basis for future decisions increases the chances that those decisions will be soundly based." (1:89-91)

The scientific uncertainty that characterizes our understanding of the vadose zone has two additional consequences: erosion of the public trust and greatly increased public expense. At sites where the remedy or containment plan ignores vadose zone processes, monitoring programs rely exclusively on the deep groundwater, which, if found to be affected would require expensive remediation efforts that could have been avoided through vadose zone monitoring and remediation.

REDUCING UNCERTAINTY

Creating a better scientific foundation for making key decisions regarding the management of contaminated sites with respect to the vadose zone is the primary goal of the R&D program suggested by the roadmap. This is true for both mid-term remediation actions and long-term stewardship activities required to protect human health and the environment from hazards remaining after cleanup is complete (5). This will require:

1) An enhanced understanding of basic subsurface process;

2) Adequate data on the extent and character of existing contamination, and the ability to monitor it effectively and;

3) The ability to translate this understanding and data into new predictive models that can minimize the technical uncertainty in environmental management decisions.

Over the next few decades, dramatic and fundamental advances in computing, communication, electronics and microengineered systems will transform many of the scientific and technical challenges we face today. With these types of advances becoming commonplace, one can envision by the year 2025:

- A new generation of microscopic sensors, the size of a grain of rice, that minimize the sensors' impacts on the measurement. These sensors will increase the density of measurement while lowering the cost of individual measurements. They will make multi-channel measurements (e.g., chemical species detection or pressure, temperature, pH or eH measurements) simultaneously in real time. These sensors may be eventually small enough to inject into the material being investigated to "illuminate" its properties (magic dust).

- Ultra-sensitive monitoring capabilities that allow investigators to determine with certainty whether or not contaminant migration is occurring on a time-scale that today would take centuries to recognize.

- Vadose zone simulation abilities comparable in their complexity, speed, and accuracy to those used to model nuclear weapons systems and explosions or

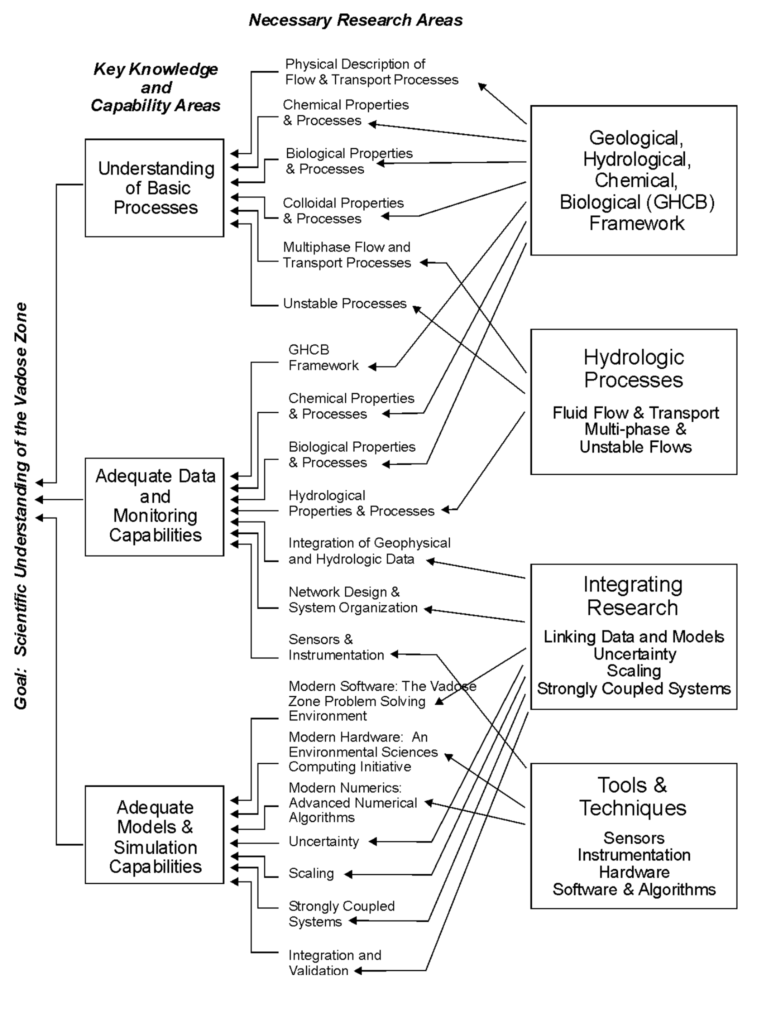

Figure 1. Connection of research priorities to topics

molecular processes in biology.

- A fundamental understanding of vadose zone properties and processes that is sufficient and robust enough so that scientific uncertainty is no longer a large component of the public and regulatory debate.

Not surprisingly, there is much overlap in the broad areas of research identified as priorities by the roadmap. This can be integrated by organizing the research required into four higher-level integrated research areas aimed at:

(1) Understanding the geological, chemical, biological and hydrological framework;

(2) Understanding fluid flow and transport;

(3) Integrating data, understanding and models within an experiment, and generalize the results beyond a single experiment or site; and

(4) Developing new tools and techniques.

These categories and their connection to the research priorities discussed are illustrated in Figure 1.

The vadose zone S&T community can organize themselves along these lines to meet the pressing need for an adequate and reliable scientific understanding of the vadose zone and develop the tools and techniques that will allow for a high degree of certainty in predictions.

Additional work to focus and sequence the research priorities identified in the roadmap will continue within the vadose zone science and technology community. These will include workshops dedicated to reaching this third level of understanding, and national meetings and technical reviews aimed at soliciting feedback from the affected stakeholders.

INTEGRATION WITHIN EXPERIMENTS AND GENERALIZATION TO OTHER SITES

Integration and integrating research is critical if the vadose zone research community is to:

- Move forward in its ability to understand the basic processes at work in the vadose zone,

- Possess the data necessary for monitoring contaminant migration and building computer simulations, and

- Adequately model and predict contaminant behavior and fluid flows.

These, when combined, will provide the scientific basis for decision-making with respect to the vadose zone. The solutions to these key integration barriers lie both in what should be addressed (technical priorities) and in how vadose zone research should be conducted (the structure and focus of the research plans and programs developed by DOE's program offices).

There is great consensus that the ability to integrate measurements and interpretation from different disciplines such as biology, geochemistry, hydrogeology, geology, geophysics, and geomechanics is fundamental to our ability to provide a solid scientific understanding of the vadose zone.

Increasing the interplay between modeling and data gathering in experimentation is another crucial element of integration in vadose zone research. Just as characterization and monitoring strategies may be improved with guidance from newer and more relevant computer models of vadose zone behaviors, the ability to discriminate among alternative conceptual models and to improve on them will depend on the validation of their predictive capabilities against characterization and monitoring data.

The ability to extrapolate results from laboratory experiments to field experiments or vice versa is one of the most pressing challenges facing vadose zone research. Solving scaling problems will be central to this ability. The addition of computer models to this picture makes scaling issues even thornier. This is because many relevant subsurface properties exhibit multiple nested scales of variability in both space and time. Simulations based on property measurements on one scale may be of little or no use to simulations on other scales affected by different flow and reactive transport processes. In this case standard theory becomes inadequate, because flow and transport at different scales requires the use of completely different mathematical models.

Uncertainties in the quantitative understanding of flow and transport of complex contaminant mixtures have many sources in data collection methodologies, modeling techniques, and gaps in the fundamental knowledge of basic properties and processes. Often, the relative contributions to uncertainty arising from these various sources are unknown. Refinement of fundamental knowledge, data collection techniques, and modeling approaches to reduce uncertainty is expensive, and the more certain we wish our monitoring and predictive capabilities to be, the more expensive the refinements become. These costs are counterbalanced by those arising from over design of engineering facilities needed to compensate for uncertainty, and by those arising from public mistrust when uncertainty is inadequately recognized and predictions fail.

CONCLUSIONS

Two challenges face the vadose zone research community: understand and reduce sources of uncertainty; and decide how much certainty is necessary to minimize over design and to avoid unpleasant surprises. For the first challenge, a next generation of characterization, monitoring and modeling capabilities is needed that provide better quantification of estimate uncertainty due to measurement errors, inversion errors, and use of estimated petrophysical relationships. We must understand how use of multiple co-located data sets reduce ambiguity and uncertainty associated with parameter estimates. Existing stochastic methodologies handle some issues involving uncertainty, but further refinement, testing, and extension of these approaches is needed, with particular regard to issues of scale. The second challenge, determining the level of scientific certainty required to make good decisions regarding the vadose zone, is not the purview of the research community alone-but will require substantial dialogue with the larger DOE, policy, and stakeholder communities.

A combination of multidisciplinary, laboratory, numerical, and field scale studies will be necessary to test specific hypotheses and relate all aspects of vadose zone behavior. Specifically, the use of integrated field experiments; organized to address vadose zone questions will be the key to fostering the integration of research approaches and knowledge necessary for revolutionary advances in the application of vadose zone research. These integrated field experiments would enable researchers of many disciplines (e.g., chemistry, biology, mathematics), with many goals (e.g., sensor, instrument or model development), and working at many scales (e.g., laboratory, bench, and field) to tackle different portions of one overarching problem.

There is much consensus within the vadose zone research community on the need for a broader and more effective means for disseminating the information that currently exists. As one participant put it, “our first steps in addressing vadose zone issues should be to apply the knowledge we have now.” To date, widespread distribution and application of this information has been greatly hampered by the lack of a convenient means for sharing vadose zone experimental data and results, and differing standard practices in data collection from site to site, and experiment to experiment.

Similarly, there is a lack of, and need for, access to unifying models that can be used for the vadose zone. To date, the flow and transport simulation capabilities that have been developed are very site-specific. The notion of a reliable and commonly used solute transport model which would allow supporting models to converge into a solution does not exist at this time, but is desirable in the long-term.

Both the vadose zone data visualization capabilities and the predictive simulations envisioned in this roadmap will require computing power on a grand scale. Modeling vadose zone behaviors is a problem of considerable difficulty. There is a need for an environmental science computing initiative, centered around a state-of-the-art massively parallel or distributed “machine” that would be available for priority use by university and national laboratory researchers working on the problems of understanding and predicting subsurface contaminant fate and transport.

The desire for a strong scientific basis for making public policy, regulatory, remediation or long-term stewardship decisions related to the vadose zone is not limited to DOE. The number of stakeholders is large. For example, other federal agencies, notably the U.S. Departments of Agriculture and Defense, the United States Geological Survey and the Environmental Protection Agency are major players. Sometimes as problem holders, sometimes as policy makers, sometimes as research sponsors, and sometimes as all three. State, local and tribal governments also have a stake in the decisions made regarding the vadose zone.

The research community is no less varied: it encompasses a wide range of academic disciplines in settings that span the public, university and private sector. Here, the interplay between regulations as drivers of technology research and development, and technology as a driver of regulation adds enormous complexity to the challenge of moving the entire field of vadose zone research forward. Public perception of risk and its acceptable levels adds unpredictability to this mix. Finally, the nature of vadose zone processes themselves: complex, incorporating large volumes of media, and undergoing transformations that may occur very rapidly or in timeframes than span centuries, do not lend themselves to quick, simple solutions.

ACKNOWLEDGEMENTS

The vadose zone science and technology roadmap represents the considerable efforts of the executive committee members and working group participants noted in Figure 2. No effort was made to attribute input from any individual contributor. I am totally responsible for this edited version of the results of the roadmap effort.

The Executive Committee	**Process Work Group**	**Characterization and Monitoring Workgroup**	**Simulation and Modeling Work Group**
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Figure 2: Executive Committee Members and Working Group Participants

FOOTNOTES

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BIOGRAPHY

Dr. Kowall is presently Program Manager at Bechtel Idaho for the DOE National Vadose Zone Science and Technology Roadmap program at the Idaho National Engineering and Environmental Laboratory (INEEL). He has fourteen years of university experience at four institutions and 20 years of senior project, program and line management experience with technology research and development companies. He has a Ph.D. in Geology from the State University of New York at Binghamton.

Dr. Kowall has served on the faculties of Brooklyn College, the University of Oklahoma and Washington and Lee University and, for seven years, as an Adjunct Lecturer in Environmental Science at Washington State University, Tri-Cities teaching environmental contaminant fate and transport.

Dr. Kowall was at Pacific Northwest National Laboratory from 1990 – 2000 where he served as Deputy Manager for Battelle's Environmental Management Organization and Manager of the Project Management Group. Dr. Kowall has been with Bechtel since February 29, 2000. He has represented the U.S. Department of Energy in two international programs and represented the U.S. at the Organization for Economic Cooperation and Development (OECD) Nuclear Energy Agency Coordinating Group on Geologic Disposal in Paris.

Dr. Kowall has represented the federal government at state, local and tribal briefings and meetings as the technical representative on several government briefing teams. Prior to his PNNL assignment he served as Principal Geologist and Project Manager for Battelle in Columbus, Ohio and Chicago, Illinois.